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# Prediction of bacterial growth on xenobiotics

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The utilisation of a given substrate leads to bacterial growth and the associated yield is normally determined experimentally. Different yield estimation methods exist based on knowledge of the Gibbs energy of reaction and the energy needed for synthesis of new biomass [1-4]. Estimating yield from thermodynamic considerations of stoichiometrically balanced reactions is typically done in biotechnology and wastewater treatment [5], an approach recently adopted by Helbling et al. [6]. More recent methods specifically incorporate detailed knowledge of the degradation pathway and bacterial metabolism to attain predictions closer to the experimentally observed yields [3]. However, this knowledge is seldom known for xenobiotics in the environment but is needed to assess the turnover leading to biomass production, i.e. for sludge production or biogenic residues. The objectives of the present study were thus to (i) formulate and use a simple quantitative structure-activity relationship to estimate a minimum growth yield under aerobic conditions and (ii) compare the estimations with experimental results from literature.

We based our estimation method on the approach suggested by Diekert [2], requiring as input just the Gibbs energy of formation of the reactants and products and a limited amount of structural data (e.g., the number of carbon atoms in the substrate). To estimate the yield, the Gibbs energy of reaction was quantified from balanced mineralisation reactions as the difference between the Gibbs energy of formation of the products and reactants.

The Gibbs energy of the mineralisation reaction can be regarded as the maximum energy released and partly captured by the biomass. The carbon present in the substrate is used for synthesis and oxidised to CO<sub>2</sub> to yield energy for anabolism. We accounted for this by specifying how much of the energy can be used as a function of the chemical structure based on general rules of microbial turnover. Thus, we obtain a minimum yield from use of the substrate as a sole source of energy and carbon. In order to test the applicability of our estimation method, we evaluated it with both simple substrates (e.g. acetate, methanol, and glyoxylate) and xenobiotics (e.g. 2,4-D, linuron, carbofuran, carbon tetrachloride, and toluene). Experimental data for the simple substrates were taken from [4], for xenobiotics from [6] and own experimental data. For simple substrates, our approach predicts yields close to experimental values and also for xenobiotics the yield predictions for most of the compounds are close to the experimentally obtained values.

Overall, with our method we were able to obtain yield predictions close to experimental values with a minimum of input information. Moreover, the estimates were comparable to estimates obtained using the method suggested by McCarty [1].

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